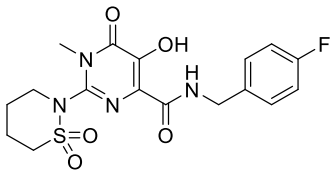
Product data sheet

MedKoo Cat#: 524519 Name: BMS-707035 CAS#: 729607-74-3 Chemical Formula: $C_{17}H_{19}FN_4O_5S$ Exact Mass: 410.10602 Molecular Weight: 410.42	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.



1. Product description:
BMS-707035 is a potent, specific, and reversible HIV-I integrase (IN) inhibitor that blocks HIV IN strand transfer activity IC50 of 15 nM. BMS-707035 binding affinity to IN is also affected by the four terminal bases at the 5' end of the pre-processed U5 long terminal repeat (LTR).

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	44.0	107.21

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	2.44 mL	12.18 mL	24.37 mL
5 mM	0.49 mL	2.44 mL	4.87 mL
10 mM	0.24 mL	1.22 mL	2.44 mL
50 mM	0.05 mL	0.24 mL	0.49 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Naidu BN, Walker MA, Sorenson ME, Ueda Y, Matiskella JD, Connolly TP, Dicker IB, Lin Z, Bollini S, Terry BJ, Higley H, Zheng M, Parker DD, Wu D, Adams S, Krystal MR, Meanwell NA. The discovery and preclinical evaluation of BMS-707035, a potent HIV-1 integrase strand transfer inhibitor. Bioorg Med Chem Lett. 2018 Jul 1;28(12):2124-2130. doi: 10.1016/j.bmcl.2018.05.027. Epub 2018 May 14. PMID: 29779976.

In vivo study

1. Naidu BN, Walker MA, Sorenson ME, Ueda Y, Matiskella JD, Connolly TP, Dicker IB, Lin Z, Bollini S, Terry BJ, Higley H, Zheng M, Parker DD, Wu D, Adams S, Krystal MR, Meanwell NA. The discovery and preclinical evaluation of BMS-707035, a potent HIV-1 integrase strand transfer inhibitor. Bioorg Med Chem Lett. 2018 Jul 1;28(12):2124-2130. doi: 10.1016/j.bmcl.2018.05.027. Epub 2018 May 14. PMID: 29779976.

7. Bioactivity
Biological target:

BMS-707035 is an HIV-1 integrase (IN) inhibitor with an IC50 value of 15 nM.

In vitro activity

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Plasma protein binding of 13a (BMS-707035) was high in all species (≥93.7%) and the compound was not overtly cytotoxic to several cell lines, with CC_{50} values of ≥45 μM.

Reference: Bioorg Med Chem Lett. 2018 Jul 1;28(12):2124-2130. https://pubmed.ncbi.nlm.nih.gov/29779976/

In vivo activity

Compound 13a (BMS-707035) was characterized as a low clearance compound in the rat, dog and monkey with moderate to long elimination half-lives in all species. The volume of distribution was low across the species, indicating that compound distribution outside of the plasma is minimal. When 13a was dosed in solution, the oral exposure was high and absolute oral bioavailabilities ranged between 56 and 129%.

Reference: Bioorg Med Chem Lett. 2018 Jul 1;28(12):2124-2130. https://pubmed.ncbi.nlm.nih.gov/29779976/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.